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Two Efficient Block Preconditioners for the Mass-Conserved Ohta-Kawasaki Equation

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Abstract. In this paper, we propose two efficient block preconditioners to solve the mass-conserved Ohta-Kawasaki equation with finite element discretization. We also study the spectral distribution of these two preconditioners, i.e., Schur complement preconditioner and the modified Hermitian and skew-Hermitian splitting (MHSS in short) preconditioner. Besides, Newton method and Picard method are used to address the implicitly nonlinear term. We rigorously analyze the convergence of Newton method. Finally, we offer numerical examples to support the theoretical analysis and indicate the efficiency of the proposed preconditioners for the mass-conserved Ohta-Kawasaki equation.

AMS subject classifications: 65F08, 65N12, 65N20, 65M60

Key words: Mass-conserved Ohta-Kawasaki equation, Newton method, Schur complement preconditioner, MHSS preconditioner.

1 Introduction

Diblock copolymers are macromolecules composed of two incompatible blocks linked together by covalent bonds. The incompatibility between the two blocks drives the system to phase separation, while the chemical bonding of the two blocks prevents the macroscopic phase separation. These competition factors lead diblock copolymers to self-assemble into a rich class of complex nanoscale structures [1,2]. Modeling and numerical simulation are effective means to investigate phase behaviors of block copolymers, such as the self-consistent field theory, and coarse-grained density functional theory [3–6].

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Among these theories, Ohta and Kawasaki [7] presented an effective free energy functional to study diblock copolymers, which can be rescaled as

$$E(u)=\int_\Omega \Big(\frac{\epsilon^2}{2}|\nabla u|^2+\frac{1}{4}(1-u^2)^2+\frac{\sigma}{2}|(-\Delta)^{-\frac{1}{2}}(u-m)|^2\Big)\,dx. \tag{1.1}$$

$u(x)$ is the order parameter that measures the order of the diblock copolymer system.

$$m=\frac{1}{|\Omega|}\int_\Omega u(x)\,dx:=\fint_\Omega u(x)\,dx$$

denotes the average mass of the melt on the domain Ω. The parameters $\epsilon\ll 1$ and σ measure the interfacial thickness in the region of pure phases and the non-local interaction potential, respectively. In the energy functional (1.1), the first term penalizes the jump in the solution, the second term favors $u=\pm 1$, and the last term penalizes variation from the mean by a long-range interaction. More physical background about the Ohta-Kawasaki free energy functional is described in [7], and corresponding mathematical theories can be found in the literature [8] and references therein.

Using the Ohta-Kawasaki free energy functional, a mass-conserved dynamic equation can be given as

$$u_t=\Delta\mu. \tag{1.2}$$

μ is the chemical potential, i.e., the variation derivative of E with respect to u

$$\mu=\frac{\delta E}{\delta u}=-\epsilon^2\Delta u-u(1-u^2)-\sigma\Delta^{-1}(u-m). \tag{1.3}$$

By introducing a new variable

$$w=-\epsilon^2\Delta u-u(1-u^2),$$

the fourth-order dynamic equation (1.2) can be split into two second-order equations on $\Omega\times[0,T]$

$$u_t-\Delta w+\sigma(u-m)=0, \tag{1.4a}$$
$$w+\epsilon^2\Delta u-u(u^2-1)=0. \tag{1.4b}$$

It is easy to verify that the energy functional (1.1) is nonincreasing in time along the solution trajectories of (1.4) with homogeneous Neumann boundary condition

$$\nabla u\cdot n=0 \quad\text{and}\quad \nabla w\cdot n=0 \quad\text{on } [0,T], \tag{1.5}$$

and the initial value $u(x,0)=u_0(x)$, $x\in\Omega$.

From the numerical computation viewpoint, it is necessary to construct an efficient numerical method to solve the gradient flow (1.4). For time discretization direction, in